

**IN THE SPECIFICATION:**

*Please delete Table 1 on pages 11-13, and replace it with the following Table:*

**Table 1**

Peptide AKAHWNDAANG (SEQ ID NO: 1)
<p><b>Modifications:</b></p> <ol style="list-style-type: none"> <li>1. acetylation; forced to occur on the amino acid at position 2 (K)</li> <li>2. methylation, variable, occurring on [CKRHDENQ] (SEQ ID NO: 2) (i.e. positions 4, 6, 7 and 10)</li> <li>3. deamidation, variable, occurring on [N] followed by a [G] (i.e. position 10)</li> <li>4. oxidation, variable, occurring on [HMW] (i.e. positions 4 and 5)</li> </ol>
<p><b>Remarks:</b></p> <p>There are the following conflict sites:</p> <ul style="list-style-type: none"> <li>• at position 4 between modifications (2) and (4)</li> <li>• at position 10, between (2) and (3)</li> </ul> <p>And no conflict sites:</p> <ul style="list-style-type: none"> <li>• at position 5, for modification (4)</li> <li>• at position 6 and 7 for (2)</li> </ul>
<pre> mass= 1195.54 : 1195.54:AK(1)AHWDAANG mass= 1209.55 : (2)@3, 1209.55:AK(1)AH(2)WDAANG mass= 1211.53 : (4)@3, 1211.53:AK(1)AH(4)WDAANG mass= 1209.55 : (2)@9, 1209.55:AK(1)AHWDAAN(2)G mass= 1223.57 : (2)@3, (2)@9, 1223.57:AK(1)AH(2)WDAAN(2)G mass= 1225.55 : (4)@3, (2)@9, 1225.55:AK(1)AH(4)WDAAN(2)G mass= 1196.52 : (3)@9, 1196.52:AK(1)AHWDAAN(3)G mass= 1210.54 : (2)@3, (3)@9, 1210.54:AK(1)AH(2)WDAAN(3)G mass= 1212.52 : (4)@3, (3)@9, 1212.52:AK(1)AH(4)WDAAN(3)G mass= 1209.55 : (2)x1, 1209.55:AK(1)AHWND(2)AANG 1209.55:AK(1)AHWN(2)DAANG mass= 1223.57 : (2)@3, (2)x1, 1223.57:AK(1)AH(2)WND(2)AANG 1223.57:AK(1)AH(2)WN(2)DAANG mass= 1225.55 : (4)@3, (2)x1, 1225.55:AK(1)AH(4)WND(2)AANG 1225.55:AK(1)AH(4)WN(2)DAANG mass= 1223.57 : (2)@9, (2)x1, 1223.57:AK(1)AHWND(2)AAN(2)G 1223.57:AK(1)AHWN(2)DAAN(2)G mass= 1237.58 : (2)@3, (2)@9, (2)x1, 1237.58:AK(1)AH(2)WND(2)AAN(2)G 1237.58:AK(1)AH(2)WN(2)DAAN(2)G mass= 1239.56 : (4)@3, (2)@9, (2)x1, 1239.56:AK(1)AH(4)WND(2)AAN(2)G 1239.56:AK(1)AH(4)WN(2)DAAN(2)G mass= 1210.54 : (3)@9, (2)x1, 1210.54:AK(1)AHWND(2)AAN(3)G 1210.54:AK(1)AHWN(2)DAAN(3)G mass= 1224.55 : (2)@3, (3)@9, (2)x1, 1224.55:AK(1)AH(2)WND(2)AAN(3)G 1224.55:AK(1)AH(2)WN(2)DAAN(3)G mass= 1226.53 : (4)@3, (3)@9, (2)x1, 1226.53:AK(1)AH(4)WND(2)AAN(3)G 1226.53:AK(1)AH(4)WN(2)DAAN(3)G mass= 1223.57 : (2)x2, 1223.57:AK(1)AHWN(2)D(2)AANG </pre>

mass= 1237.58 : (2)@3, (2)x2,  
1237.58:AK(1)AH(2)WN(2)D(2)AANG  
mass= 1239.56 : (4)@3, (2)x2,  
1239.56:AK(1)AH(4)WN(2)D(2)AANG  
mass= 1237.58 : (2)@9, (2)x2,  
1237.58:AK(1)AHWN(2)D(2)AAN(2)G  
mass= 1251.6 : (2)@3, (2)@9, (2)x2,  
1251.6:AK(1)AH(2)WN(2)D(2)AAN(2)G  
mass= 1253.58 : (4)@3, (2)@9, (2)x2,  
1253.58:AK(1)AH(4)WN(2)D(2)AAN(2)G  
mass= 1224.55 : (3)@9, (2)x2,  
1224.55:AK(1)AHWN(2)D(2)AAN(3)G  
mass= 1238.57 : (2)@3, (3)@9, (2)x2,  
1238.57:AK(1)AH(2)WN(2)D(2)AAN(3)G  
mass= 1240.55 : (4)@3, (3)@9, (2)x2,  
1240.55:AK(1)AH(4)WN(2)D(2)AAN(3)G  
mass= 1211.53 : (4)x1,  
1211.53:AK(1)AHW(4)NDAANG  
mass= 1225.55 : (2)@3, (4)x1,  
1225.55:AK(1)AH(2)W(4)NDAANG  
mass= 1227.53 : (4)@3, (4)x1,  
1227.53:AK(1)AH(4)W(4)NDAANG  
mass= 1225.55 : (2)@9, (4)x1,  
1225.55:AK(1)AHW(4)NDAAN(2)G  
mass= 1239.56 : (2)@3, (2)@9, (4)x1,  
1239.56:AK(1)AH(2)W(4)NDAAN(2)G  
mass= 1241.54 : (4)@3, (2)@9, (4)x1,  
1241.54:AK(1)AH(4)W(4)NDAAN(2)G  
mass= 1212.52 : (3)@9, (4)x1,  
1212.52:AK(1)AHW(4)NDAAN(3)G  
mass= 1226.53 : (2)@3, (3)@9, (4)x1,  
1226.53:AK(1)AH(2)W(4)NDAAN(3)G  
mass= 1228.51 : (4)@3, (3)@9, (4)x1,  
1228.51:AK(1)AH(4)W(4)NDAAN(3)G  
mass= 1225.55 : (2)x1, (4)x1,  
1225.55:AK(1)AHW(4)ND(2)AANG  
1225.55:AK(1)AHW(4)N(2)DAANG  
mass= 1239.56 : (2)@3, (2)x1, (4)x1,  
1239.56:AK(1)AH(2)W(4)ND(2)AANG  
1239.56:AK(1)AH(2)W(4)N(2)DAANG  
mass= 1241.54 : (4)@3, (2)x1, (4)x1,  
1241.54:AK(1)AH(4)W(4)ND(2)AANG  
1241.54:AK(1)AH(4)W(4)N(2)DAANG  
mass= 1239.56 : (2)@9, (2)x1, (4)x1,  
1239.56:AK(1)AHW(4)ND(2)AAN(2)G  
1239.56:AK(1)AHW(4)N(2)DAAN(2)G  
mass= 1253.58 : (2)@3, (2)@9, (2)x1, (4)x1,  
1253.58:AK(1)AH(2)W(4)ND(2)AAN(2)G  
1253.58:AK(1)AH(2)W(4)N(2)DAAN(2)G  
mass= 1255.56 : (4)@3, (2)@9, (2)x1, (4)x1,  
1255.56:AK(1)AH(4)W(4)ND(2)AAN(2)G  
1255.56:AK(1)AH(4)W(4)N(2)DAAN(2)G  
mass= 1226.53 : (3)@9, (2)x1, (4)x1,  
1226.53:AK(1)AHW(4)ND(2)AAN(3)G  
1226.53:AK(1)AHW(4)N(2)DAAN(3)G  
mass= 1240.55 : (2)@3, (3)@9, (2)x1, (4)x1,  
1240.55:AK(1)AH(2)W(4)ND(2)AAN(3)G  
1240.55:AK(1)AH(2)W(4)N(2)DAAN(3)G  
mass= 1242.53 : (4)@3, (3)@9, (2)x1, (4)x1,  
1242.53:AK(1)AH(4)W(4)ND(2)AAN(3)G  
1242.53:AK(1)AH(4)W(4)N(2)DAAN(3)G  
mass= 1239.56 : (2)x2, (4)x1,  
1239.56:AK(1)AHW(4)N(2)D(2)AANG  
mass= 1253.58 : (2)@3, (2)x2, (4)x1,  
1253.58:AK(1)AH(2)W(4)N(2)D(2)AANG  
mass= 1255.56 : (4)@3, (2)x2, (4)x1,  
1255.56:AK(1)AH(4)W(4)N(2)D(2)AANG  
mass= 1253.58 : (2)@9, (2)x2, (4)x1,  
1253.58:AK(1)AHW(4)N(2)D(2)AAN(2)G  
mass= 1267.59 : (2)@3, (2)@9, (2)x2, (4)x1,  
1267.59:AK(1)AH(2)W(4)N(2)D(2)AAN(2)G  
mass= 1269.57 : (4)@3, (2)@9, (2)x2, (4)x1,  
1269.57:AK(1)AH(4)W(4)N(2)D(2)AAN(2)G  
mass= 1240.55 : (3)@9, (2)x2, (4)x1,  
1240.55:AK(1)AHW(4)N(2)D(2)AAN(3)G  
mass= 1254.56 : (2)@3, (3)@9, (2)x2, (4)x1,  
1254.56:AK(1)AH(2)W(4)N(2)D(2)AAN(3)G  
mass= 1256.54 : (4)@3, (3)@9, (2)x2, (4)x1,  
1256.54:AK(1)AH(4)W(4)N(2)D(2)AAN(3)G

*Please delete Table 2 on pages 15-16, and replace it with the following Table:*

**Table 2**

**(SEQ ID NOS 3-31, respectively in order of appearance)**

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0 ACET_nterm (Acetylation_nterm) [ACDEFGHIKLMNPQRSTVWY:~NKHFWY:ACDEFGHIKLMNPQRSTVWY]
T---F 42.0106:42.0373

1 ACET_core (Acetylation_core) [ACDEFGHIKLMNPQRSTVWY:K:ACDEFGHIKLMNPQRSTVWY]
F---F 42.0106:42.0373

2 PHOS (Phosphorylation) [ACDEFGHIKLMNPQRSTVWY:DHSTY:ACDEFGHIKLMNPQRSTVWY]
F---F 79.9663:79.9799

3 AMID (Amidation) [ACDEFGHIKLMNPQRSTVWY:ACDEFGHIKLMNPQRSTVWY:G]
F---T -0.984:-0.9847

4 BIOT (Biotin) [ACDEFGHIKLMNPQRSTVWY:K:ACDEFGHIKLMNPQRSTVWY]
F---T 226.078:226.293

5 CAM_nterm (Carbamylation_nterm)
[ACDEFGHIKLMNPQRSTVWY:ACDEFGHIKLMNPQRSTVWY:ACDEFGHIKLMNPQRSTVWY]
T---F 43.0058:43.025

6 CAM_core (Carbamylation_core) [ACDEFGHIKLMNPQRSTVWY:K:ACDEFGHIKLMNPQRSTVWY]
F---F 43.0058:43.025

7 CARB (Carboxylation) [ACDEFGHIKLMNPQRSTVWY:EN:ACDEFGHIKLMNPQRSTVWY]
F---F 43.9898:44.0098

8 PYRR (Pyrrolidone_carboxylic_acid) [ACDEFGHIKLMNPQRSTVWY:Q:ACDEFGHIKLMNPQRSTVWY]
T---F -17.0266:-17.0306

9 HYDR (Hydroxylation) [ACDEFGHIKLMNPQRSTVWY:DKNP:ACDEFGHIKLMNPQRSTVWY]
F---F 15.9949:15.9994

10 GGLU (Gamma-carboxyglutamic_acid) [ACDEFGHIKLMNPQRSTVWY:E:ACDEFGHIKLMNPQRSTVWY]
F---F 43.9898:44.0098

11 METH_nterm (Methylation_nterm) [ACDEFGHIKLMNPQRSTVWY:AP:ACDEFGHIKLMNPQRSTVWY]
T---F 14.0157:14.0269

12 METH_core (Methylation_core) [ACDEFGHIKLMNPQRSTVWY:CDEHKNQR:ACDEFGHIKLMNPQRSTVWY]
F---F 14.0157:14.0269

13 DIMETH_nterm (Di-Methylation_nterm) [ACDEFGHIKLMNPQRSTVWY:AP:ACDEFGHIKLMNPQRSTVWY]
T---F 28.0314:28.0538

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**Table 2 continued.**

14	DIMETH_core (Di-Methylation_core)	[ACDEFGHIKLMNPQRSTVWY:CDEHKNQR:ACDEFGHIKLMNPQRSTVWY]	F---F 28.0314:28.0538
15	TRIMETH_nterm (Tri-Methylation_nterm)	[ACDEFGHIKLMNPQRSTVWY:AP:ACDEFGHIKLMNPQRSTVWY]	T---F 42.0471:42.0807
16	TRIMETH_core (Tri-Methylation_core)	[ACDEFGHIKLMNPQRSTVWY:CDEHKNQR:ACDEFGHIKLMNPQRSTVWY]	F---F 42.0471:42.0807
17	SULF_nterm (Sulfation_nterm)	[ACDEFGHIKLMNPQRSTVWY:ACDEFGHIKLMNPQRSTVWY:ACDEFGHIKLMNPQRSTVWY]	T---F 79.9568:80.0642
18	SULF (Sulfation_core)	[ACDEFGHIKLMNPQRSTVWY:Y:ACDEFGHIKLMNPQRSTVWY]	F---F 79.9568:80.0642
19	FORM (Formylation)	[ACDEFGHIKLMNPQRSTVWY:ACDEFGHIKLMNPQRSTVWY:ACDEFGHIKLMNPQRSTVWY]	T---F 27.9949:28.0104
20	DEAM_N (Deamidation_N)	[ACDEFGHIKLMNPQRSTVWY:N:G]	F---F 0.984:0.9847
21	DEAM_Q (Deamidation_Q)	[ACDEFGHIKLMNPQRSTVWY:Q:ACDEFGHIKLMNPQRSTVWY]	F---F 0.984:0.9847
22	Oxydation (Oxydation)	[ACDEFGHIKLMNPQRSTVWY:HMW:ACDEFGHIKLMNPQRSTVWY]	F---F 15.9949:15.999
23	Cys_CM (Carboxymethyl_cysteine)	[ACDEFGHIKLMNPQRSTVWY:C:ACDEFGHIKLMNPQRSTVWY]	F---F 58.0055:58.0367
24	Cys_CAM (Carboxyamidomethyl_cysteine)	[ACDEFGHIKLMNPQRSTVWY:C:ACDEFGHIKLMNPQRSTVWY]	F---F 57.0215:57.052
25	Cys_PE (Pyridyl-ethyl_cysteine)	[ACDEFGHIKLMNPQRSTVWY:C:ACDEFGHIKLMNPQRSTVWY]	F---F 105.058:105.145
26	Cys_PAM (Propionamide_cysteine)	[ACDEFGHIKLMNPQRSTVWY:C:ACDEFGHIKLMNPQRSTVWY]	F---F 71.0371:71.0788
27	MSO (Methionine_sulfoxide)	[ACDEFGHIKLMNPQRSTVWY:M:ACDEFGHIKLMNPQRSTVWY]	F---F 15.9949:15.9994
28	HSL (Homoserine_Lactone)	[ACDEFGHIKLMNPQRSTVWY:S:ACDEFGHIKLMNPQRSTVWY]	F---F 12.9617:13.0189

*Please delete the paragraph on page 17, lines 9-14, and replace it with the following paragraph:*

Table 4 is the theoretical MS/MS spectrum of peptide tryptic FPNCYQKPCNR (**SEQ ID NO: 32**). Modification Cys\_CAM (iodoacetamide, +57Da) used to break di-sulfur bonds have been considered as a variable modification. The rule is that every cysteine (C) can be modified. The total mass of the peptide is in the column labeled as "Total". The two cases where one cysteine only is modified share the same total mass. As the fragment masses are needed, the exact location of the modifications is necessary.

Please delete Table 3 on page 19, and replace it with the following Table:

Table 3

(SEQ ID NO: 33)

	E	P	C	V	E	S	L	V	D	L	Y	F	Q	T	I	P	D	Y	G	K
<b>a</b>	102	199	359	458	587	674	787	886	1001	1115	1278	1425	1554	1655	1768	1865	1980	2143	2200	2328
<b>a-NH3*</b>	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	1537	1638	1751	1848	1963	2126	2183	2311
	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	2294
<b>a-H2O*</b>	-1	-1	-1	-1	-1	656	769	868	983	1097	1260	1407	1536	1637	1750	1847	1962	2125	2182	2310
	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	1619	1732	1829	1944	2107	2164	2292
<b>a++</b>	52	100	180	230	294	338	394	444	501	558	639	713	777	828	884	933	990	1072	1101	1165
<b>b</b>	130	227	387	486	615	702	815	914	1029	1143	1306	1453	1582	1683	1796	1893	2008	2171	2228	2356
<b>b-NH3*</b>	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	1565	1666	1779	1876	1991	2154	2211	2339
	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	2322
<b>b-H2O*</b>	-1	-1	-1	-1	-1	684	797	896	1011	1125	1288	1435	1564	1665	1778	1875	1990	2153	2210	2338
	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	1647	1760	1857	1972	2135	2192	2320
<b>b++</b>	66	114	194	244	308	352	408	458	515	572	653	727	791	842	898	947	1004	1086	1115	1179
<b>y</b>	2374	2245	2148	1988	1889	1760	1673	1560	1461	1346	1233	1070	922	793	692	579	482	367	204	147
<b>y-NH3*</b>	2357	2228	2131	1971	1872	1743	1656	1543	1444	1329	1216	1052	905	776	675	562	465	350	187	130
	2340	2211	2114	1954	1855	1726	1639	1526	1427	1312	1199	1035	888	-1	-1	-1	-1	-1	-1	-1
<b>y-H2O*</b>	2356	2227	2130	1970	1871	1742	1655	1542	1443	1328	1215	1052	904	775	-1	-1	-1	-1	-1	-1
	2338	2209	2112	1952	1853	1724	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
<b>y++</b>	1188	1123	1075	995	945	880	837	780	731	673	617	535	462	397	347	290	242	184	103	74

*Please delete Table 4 on page 20, and replace it with the following Table:*

**Table 4**

**(SEQ ID NO: 32)**

	<b>F</b>	<b>P</b>	<b>N</b>	<b>C</b>	<b>Y</b>	<b>Q</b>	<b>K</b>	<b>P</b>	<b>C</b>	<b>N</b>	<b>R</b>	<b>Total</b>
<b>b</b>	148.1	245.1	359.2	462.2	625.2	753.3	881.4	978.5	1081.5	1195.5	1351.6	1368.6
<b>y</b>	1369.5	1222.55	1125.5	1011.5	908.4	745.4	617.3	489.2	392.2	289.2	175.1	
	<b>F</b>	<b>P</b>	<b>N</b>	<b>C*</b>	<b>Y</b>	<b>Q</b>	<b>K</b>	<b>P</b>	<b>C</b>	<b>N</b>	<b>R</b>	<b>Total</b>
<b>b</b>	148.1	245.1	359.2	519.2	682.3	810.3	938.4	1035.5	1138.5	1252.5	1408.6	1425.6
<b>y</b>	1426.6	1279.6	1182.5	1068.5	908.4	745.4	617.3	489.2	392.2	289.2	175.1	
	<b>F</b>	<b>P</b>	<b>N</b>	<b>C</b>	<b>Y</b>	<b>Q</b>	<b>K</b>	<b>P</b>	<b>C*</b>	<b>N</b>	<b>R</b>	<b>Total</b>
<b>b</b>	148.1	245.1	359.2	462.2	625.2	753.3	881.4	978.5	1138.5	1252.5	1408.6	1425.6
<b>y</b>	1426.6	1279.6	1182.5	1068.5	965.5	802.4	674.4	546.3	449.2	289.2	175.1	
	<b>F</b>	<b>P</b>	<b>N</b>	<b>C*</b>	<b>Y</b>	<b>Q</b>	<b>K</b>	<b>P</b>	<b>C*</b>	<b>N</b>	<b>R</b>	<b>Total</b>
<b>b</b>	148.1	245.1	359.2	519.2	682.3	810.3	938.4	1035.5	1195.5	1309.6	1465.7	1482.7
<b>y</b>	1483.7	1336.6	1239.5	1125.5	965.5	802.4	674.4	546.3	449.2	289.2	175.1	

Please delete Table 5 on page 23, and replace it with the following Table:

**Table 5**

<b>Usual tryptic cleavage rule:</b> trypsin cleaves after every occurrence of K or R except if they are followed by P.
<b>Usual rule for missed cleavage:</b> every cleavage site is considered as a possible missed cleavage site.
<b>Adapted rule (Thiede et al. 2000):</b> missed cleavages are only possible in the following situations: <ol style="list-style-type: none"> <li>1. K or R followed by P</li> <li>2. K or R followed by K or R</li> <li>3. K or R preceded by K or R</li> <li>4. K or R followed by D or E</li> <li>5. K or R preceded by D or E</li> </ol>
<b>Example:</b> sequence <b>ATGWRQSTRDASYT (SEQ ID NO: 34)</b>  Usual rule yields peptides: ATGWR ( <b>SEQ ID NO: 35</b> ), QSTR ( <b>SEQ ID NO: 36</b> ), DASYT ( <b>SEQ ID NO: 37</b> ), <u>ATGWRQSTR</u> (1) ( <b>SEQ ID NO: 38</b> ), <u>QSTRDASYT</u> (1) ( <b>SEQ ID NO: 39</b> ), <u>ATGWRQSTRDASYT</u> (2) ( <b>SEQ ID NO: 34</b> ). Adapted rule yields peptides: ATGWR ( <b>SEQ ID NO: 35</b> ), QSTR ( <b>SEQ ID NO: 36</b> ), DASYT ( <b>SEQ ID NO: 37</b> ), <u>QSTRDASYT</u> (1) ( <b>SEQ ID NO: 39</b> ).  <i>The peptides with missed cleavages are underlined with the number of missed cleavages (k) in parentheses.</i>



Please delete Table 6 on pages 41-42, and replace it with the following Table:

**Table 6**

<p>FRAGMENT PROBABILITIES PER AA CLASS</p> <p>oneAAClass aa="AFHILMVWY" (<u>SEQ ID NO: 40</u>) charge="2" nTerm="yes"</p> <p>oneAAClass aa="CDEGNQST" (<u>SEQ ID NO: 41</u>) charge="2" nTerm="yes"</p> <p>oneAAClass aa="KPR" charge="2" nTerm="yes"</p> <p>oneAAClass aa="HP" charge="2" nTerm="no"</p> <p>oneAAClass aa="ACFIMDEGLNQSTVWY" (<u>SEQ ID NO: 42</u>) charge="2" nTerm="no"</p> <p>oneAAClass aa="KR" charge="2" nTerm="no"</p> <p>fragType="a" aaClass="AFHILMVWY" (<u>SEQ ID NO: 40</u>) foundProb="0.174985"</p> <p>notFoundProb="0.0796809"</p> <p>fragType="a-NH3" aaClass="AFHILMVWY" (<u>SEQ ID NO: 40</u>) foundProb="0.184976"</p> <p>notFoundProb="0.0891291"</p> <p>fragType="b" aaClass="AFHILMVWY" (<u>SEQ ID NO: 40</u>) foundProb="0.572251"</p> <p>notFoundProb="0.0924224"</p> <p>fragType="b" aaClass="CDEGNQST" (<u>SEQ ID NO: 41</u>) foundProb="0.464668"</p> <p>notFoundProb="0.0918588"</p> <p>fragType="b" aaClass="KPR" foundProb="0.315322" notFoundProb="0.198784"</p> <p>fragType="b-H2O" aaClass="AFHILMVWY" (<u>SEQ ID NO: 40</u>) foundProb="0.556841"</p> <p>notFoundProb="0.099369"</p> <p>fragType="b-H2O" aaClass="CDEGNQST" (<u>SEQ ID NO: 41</u>) foundProb="0.413524"</p> <p>notFoundProb="0.0908845"</p> <p>fragType="b-H2O" aaClass="KPR" foundProb="0.191116" notFoundProb="0.123449"</p> <p>fragType="b-NH3" aaClass="AFHILMVWY" (<u>SEQ ID NO: 40</u>) foundProb="0.342007"</p> <p>notFoundProb="0.0960211"</p> <p>fragType="b-NH3" aaClass="CDEGNQST" (<u>SEQ ID NO: 41</u>) foundProb="0.300601"</p> <p>notFoundProb="0.0914023"</p> <p>fragType="y" aaClass="HP" foundProb="0.72187" notFoundProb="0.0758288"</p> <p>fragType="y" aaClass="ACFIMDEGLNQSTVWY" (<u>SEQ ID NO: 42</u>) foundProb="0.654344"</p> <p>notFoundProb="0.074072"</p> <p>fragType="y++" aaClass="HP" foundProb="0.136688" notFoundProb="0.0504078"</p> <p>fragType="y++-H2O" aaClass="HP" foundProb="0.152157" notFoundProb="0.0763926"</p> <p>fragType="y++-H2O" aaClass="KR" foundProb="0.219081" notFoundProb="0.0591648"</p> <p>fragType="y++-NH3" aaClass="HP" foundProb="0.162445" notFoundProb="0.0613693"</p> <p>fragType="y-H2O" aaClass="HP" foundProb="0.492051" notFoundProb="0.095759"</p> <p>fragType="y-H2O" aaClass="ACFIMDEGLNQSTVWY" (<u>SEQ ID NO: 42</u>) foundProb="0.382798"</p> <p>notFoundProb="0.11102"</p> <p>fragType="y-H2O" aaClass="KR" foundProb="0.261484" notFoundProb="0.0935407"</p> <p>fragType="y-NH3" aaClass="HP" foundProb="0.227974" notFoundProb="0.0803569"</p> <p>fragType="y-NH3" aaClass="ACFIMDEGLNQSTVWY" (<u>SEQ ID NO: 42</u>) foundProb="0.229808"</p> <p>notFoundProb="0.079139"</p>
<p>INTENSITY (5 bins, based on the rank, random probability is 0.2)</p> <p>fragType="b" matchProb="0.0668139 0.0796404 0.113967 0.193713 0.546128"</p> <p>fragType="b++" matchProb="0.11316 0.122381 0.135792 0.198659 0.432104"</p> <p>fragType="b-NH3" matchProb="0.127768 0.141787 0.165525 0.246296 0.31942"</p> <p>fragType="b-H2O" matchProb="0.0952763 0.106863 0.140196 0.240998 0.417112"</p> <p>fragType="y" matchProb="0.0323419 0.0365731 0.0575199 0.108714 0.765061"</p> <p>fragType="y++" matchProb="0.103134 0.127551 0.152697 0.216837 0.401603"</p> <p>fragType="y-NH3" matchProb="0.151402 0.163136 0.189537 0.24837 0.24837"</p> <p>fragType="y-H2O" matchProb="0.104856 0.109809 0.139647 0.210921 0.435371"</p>
<p>CONSECUTIVE FRAGMENT MATCHES</p> <p>name="hmmJ, alternative: (+),b,b-H2O,b-NH3" order="2"</p> <p>States:</p> <p>oneState name="S"</p> <p>oneState name="S1"</p> <p>oneState name="S2"</p> <p>Emissions:</p> <p>oneEmission name="s"</p>

```
oneEmission name="m"
oneEmission name="f"
Links:
  oneLink from="S" to="S1" prob="1"
  oneLink from="S1" to="S1" prob="0.642728"
  oneLink from="S1" to="S2" prob="0.357272"
  oneLink from="S2" to="S1" prob="0.0666977"
  oneLink from="S2" to="S2" prob="0.933302"
Emits:
  oneEmit state="S" emit="s" prob="1"
  oneEmit state="S1" emit="m" prob="0.00347297"
  oneEmit state="S1" emit="f" prob="0.996527"
  oneEmit state="S2" emit="m" prob="0.854912"
  oneEmit state="S2" emit="f" prob="0.145088"

name="hmmJ, null: (+),b,b-H2O,b-NH3" order="2"
States:
  oneState name="S"
  oneState name="S1"
  oneState name="S2"
Emissions:
  oneEmission name="s"
  oneEmission name="m"
  oneEmission name="f"
Links:
  oneLink from="S" to="S1" prob="1"
  oneLink from="S1" to="S1" prob="0.775506"
  oneLink from="S1" to="S2" prob="0.224494"
  oneLink from="S2" to="S1" prob="0.0477655"
  oneLink from="S2" to="S2" prob="0.952234"
Emits:
  oneEmit state="S" emit="s" prob="1"
  oneEmit state="S1" emit="m" prob="0.00110366"
  oneEmit state="S1" emit="f" prob="0.998896"
  oneEmit state="S2" emit="m" prob="0.3068"
  oneEmit state="S2" emit="f" prob="0.6932"

name="hmmJ, alternative: (-),y,y-H2O,y-NH3" order="2"
States:
  oneState name="S"
  oneState name="S1"
  oneState name="S2"
Emissions:
  oneEmission name="s"
  oneEmission name="m"
  oneEmission name="f"
Links:
  oneLink from="S" to="S1" prob="1"
  oneLink from="S1" to="S1" prob="0.591697"
  oneLink from="S1" to="S2" prob="0.408303"
  oneLink from="S2" to="S1" prob="0.124842"
  oneLink from="S2" to="S2" prob="0.875158"
Emits:
  oneEmit state="S" emit="s" prob="1"
  oneEmit state="S1" emit="m" prob="0.0463787"
  oneEmit state="S1" emit="f" prob="0.953621"
  oneEmit state="S2" emit="m" prob="0.968159"
  oneEmit state="S2" emit="f" prob="0.0318407"

name="hmmJ, null: (-),y,y-H2O,y-NH3" order="2"
States:
  oneState name="S"
  oneState name="S1"
  oneState name="S2"
Emissions:
  oneEmission name="s"
  oneEmission name="m"
  oneEmission name="f"
Links:
  oneLink from="S" to="S1" prob="1"
```

```
oneLink from="S1" to="S1" prob="0.770504"  
oneLink from="S1" to="S2" prob="0.229496"  
oneLink from="S2" to="S1" prob="0.136185"  
oneLink from="S2" to="S2" prob="0.863815"  
Emits:  
oneEmit state="S" emit="s" prob="1"  
oneEmit state="S1" emit="m" prob="0.0202632"  
oneEmit state="S1" emit="f" prob="0.979737"  
oneEmit state="S2" emit="m" prob="0.31142"  
oneEmit state="S2" emit="f" prob="0.68858"
```

*Please delete paragraph [0071] that extends from page 27 to page 28, and replace it with the following paragraph:*

[0071]  $F$  is a fragment match, *i.e.* the match restricted to what concerns the fragments. Typically, when a peptide match is observed, the theoretical MS/MS spectrum is computed with possible modifications  $W$  included to match the peptide mass. See Baker & Clauser (Baker, P. and Clauser, K. *MS-Product*, part of the Protein Prospector suite at <http://prospector.ucsf.edu/>) for theoretical MS/MS spectrum computation. The fragment match is then composed of the experimental fragment masses that are close enough to theoretical fragment masses:

$$F = \{(f_j, \text{int}(f_j), \text{series}(f_j), \text{pos}(f_j), m_{t,j})\}, j \in J$$

where  $J$  is a set of indices used for indexing the experimental fragment masses  $f_j$  that are close enough to a theoretical fragment mass. Assuming that  $m_{t,j}$  is the theoretical fragment mass; hence an experimental mass  $f_j$  is close enough to a theoretical mass if  $|f_j - m_{t,j}| \leq D_f$  or, in case we give the tolerance in ppm, if  $10^6 |f_j - m_{t,j}| / (0.5(f_j + m_{t,j})) \leq D_f$  or, in case of a non-symmetric tolerance,  $f_j \in D_f(m_{t,j})$ . The theoretical mass  $m_{t,j}$  corresponds to the amino acid at position  $\text{pos}(f_j)$  in the peptide sequence and ion series  $\text{series}(f_j) \in S$ . The intensity of the experimental signal  $f_j$  is  $\text{int}(f_j)$ . See Tables 3 and 4 for an example. The theoretical MS/MS spectrum of a peptide depends on the ion series ( $S$ ) and on the peptide modifications ( $W$ ), then  $F$  is written as  $F(D_f, S, W)$ . The information about intensity contained in tuple  $F$  may be removed. The information per individual fragment may be augmented by extra information provided by the signal processing software (peak detection) like peak width, signal to noise, quality of fit with a peptide signal theoretical pattern, etc. Hence a more complete version of  $F$  is

$$F = \{(f_j, \text{int}(f_j), \text{width}(f_j), \text{sn}(f_j), \text{fit}(f_j), \text{series}(f_j), \text{pos}(f_j), m_{t,j})\}, j \in J.$$